Optoelectronic Property Evaluation of Synthesized Organic Dyes using DFT/TDDFT Computational Strategies

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Computational calculations play an important role in designing new sensitizers, which provide an insightful understanding of the correlation between optical properties and the chemical structures of the dyes. In this study, series of synthesized organic compounds: Anthracene-9-ylethylanthracene-9-carboxylate, Pyrene-1-ylmethyl-4-bromobenzoate, Pyren-1-ylmethyl-4-(9-hexyl-6-{4-[(pyren-1-ylmethoxy) carbonyl] phenyl}-9H carbazole-3-yl), 3, 6-di (anthracene-9-yl)-9-hexyl-9H-carbazole,9-10-di(pyren-1-yl)anthracene,2,5-bis(anthracene-9-yl)-3-hexylthophene,and 3,6-bis(phenanthren-9-yl)-9-phenyl-9H-carbazol were studied by both density functional theory (DFT) and time dependent density functional theory (TDDFT) calculations using Gaussian 09 software. The solvation effect of acetonitrile solution is included in the calculations of molecular structural properties, electron bands and optical excitation spectra properties. Results reveal that 3,6-bis(phenanthren-9-yl)-9-phenyl-9H-carbazol is a more promising candidate for efficient dye-sensitized nanostructured solar cells (DSSCs), with relatively smaller energy gap and satisfied levels of series of optoelectronic properties. The results of this study is a good starting point for molecular level science of low-cost metal-free organic sensitizers based on organic dyes.

Keywords: Optoelectronic devices, organic dyes, DFT, TDDFT, Gaussian 09